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A FE^2 modelling approach to hydromechanical coupling in cracking-induced localization problems

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ABSTRACT

An approach to multiscale modelling of the hydro-mechanical behaviour of geomaterials in the framework of computational homogenization is presented. At the micro level a representative elementary volume (REV) is used to model the material behaviour based on the interaction between a solid skeleton and a pore fluid to provide the global material responses and associated stiffness matrices. Computational homogenization is used to retrieve these stiffness matrices from the micro level. The global response to deformation of the REV serves as an implicit constitutive law for the macroscale. On the macroscale, a poro-mechanical continuum is defined with coupled hydro-mechanical behaviour, relying on the constitutive relations obtained from the modelling at the microscale. This double scale approach is applied in the simulation of a biaxial deformation tests and the response at the macro level is related to the micro-mechanical behaviour. Hydromechanical coupling is studied as well as material anisotropy. To be able to study localization of strain, the doublescale approach is coupled with a local second gradient paradigm to maintain mesh objectivity when shear bands develop.

1. Introduction

The classical approach to modelling hydromechanical coupling in materials is the poromechanical description, founded on the pioneering work of Biot (1941), in which a solid and a fluid continuum exist at the same material point and the behaviour of both continua and their interaction are modelled by phenomenological relations (for details, developments and a review see Coussy (1995) and Schanz (2009)). The phenomenological relations of the poromechanical description are supposed to correctly represent the interaction between the solid skeleton and the pore fluid, that could be identified at a microscopic scale. These relations are readily available for cases in which material properties are constant, but for more complex behaviour, the formulation of constitutive relations and their implementation in numerical methods becomes more and more complex. An alternative approach to deriving the macroscale constitutive relations is to start from the underlying microstructural description, for which the different components of the material can be modelled explicitly and the interaction of the constituents can be defined based on physical considerations.

In this work, the framework of computational homogenization is used in the finite element squared (FE^2) method. On a microscale level, the microstructure of the material is modelled in a representative elementary volume (REV), of which the homogenized response serves as a numerical constitutive relations in the macroscale continuum. This framework was initially introduced for the modelling of microstructural solids of different nature (Feyel and Chaboche, 2000; Kouznetsova et al., 2001; Miehe and Koch, 2002; Terada and Kikuchi, 1995, see also Schröder, 2014 for an extensive overview) and later extended to multiphysics couplings, starting with thermomechanical coupling by Özdemir et al. (2008a); 2008b). Aspects of hydromechanical coupling were studied using computational homogenization by Massart (Massart and Selvadurai, 2012; 2014), and doublescale computations with computational homogenization of hydromechanical coupled behaviour were studied in Mercatoris et al. (2014) and Jänicke et al. (2015).

These methods all describe first-order computational homogenization schemes, taking into account only the first gradient of the kinematics fields, which allows the full incorporation of the separation of scales. This means that the length scale of the kinematical gradients at the macroscale is much larger than the microstructural REV, such that the REV represents the material point behaviour. The result of the separation of scales is that no

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macroscopic length scale can be taken into account and the method is limited to the classical continuum mechanics theory (Geers et al., 2010). As a result, a continuum approach has to be maintained at the macroscale throughout the computation. To overcome these limitations of the classical continuum theory, the method was extended to second-order computational homogenization (Feyel, 2003; Kouznetsova et al., 2004), deriving the classical part of the constitutive behaviour as well as the higher gradient part, thereby directly linking the length scales between micro and macroscale. With these enrichments, objectivity of the solutions with respect to the mesh was restored at the cost of losing the separation of scales.

Additional approaches were presented for micromorphic continua (Jänicke et al., 2009), while others have abandoned the macroscale continuum formulation and introduced discontinuous modes of deformation (Coenen et al., 2011a; Mercatoris and Massart, 2011; Nguyen et al., 2011; Toro et al., 2014). However, the application of these discontinuous modes of deformation at the macroscale could lead to complications in case of multiphase couplings and the restriction to a macroscale continuum is therefore preferred in this work.

At the macroscale, difficulties arise in the classical formulation when softening response is to be considered, and the well-known mesh-sensitivity appears with the loss of ellipticity of the equilibrium equations (Pijaudier-Chabot and Bažant, 1987). To restore the well-posedness of the macroscale problem, an enrichment of the kinematical constraints is required. This enrichment has to allow the use of any classical constitutive relation, both for the mechanical and the hydraulic behaviour and its coupling, since the computational homogenization will provide a constitutive relation in the most general form.

In this work a computational homogenization approach is introduced for the homogenization of microscale solid-fluid interaction to obtain a macroscale poromechanical description. The microscale model is based on the work of Frey et al. (2012). It describes the interaction between the solid skeleton and pore fluid in a REV, without relying on phenomenological coupling relations at the microscale. For upscaling the hydromechanical coupled response to kinematic loading of the REV, the framework of computational homogenization (Kouznetsova et al., 2001) is extended to take into account the hydromechanical coupled behaviour. The resulting numerical constitutive relation is coupled with a local second gradient paradigm for hydromechanical coupling (Collin et al., 2006). With the decomposition assumption between first and second gradient parts of the constitutive equations (Chambon et al., 2001), the continuum can be combined with any classical constitutive relation for hydromechanical coupling.

The paper is structured as follows; Section 2 presents the macroscale formulation of the poromechanical continuum with the local second gradient model. Section 3 introduces the framework for the REV derived from the assumption of local periodicity and introduces the micromechanical model. Section 4 provides the formulation of the computational homogenization for hydromechanical coupling based on the Hill-Mandel macro-homogeneity principle to derive the definitions of homogenized macro response. An example of the application of the model is given in Section 5 on the modelling of biaxial compression under transient conditions. The paper closes with some concluding remarks in Section 6.

2. Macroscale formulation of the saturated poromechanical continuum in finite deformation

As it is the ambition to apply the method on localization problems with material softening, an enhancement of the macroscale continuum is required to maintain the objectivity of the macroscale formulation in the softening domain. Many regularization methods were proposed for this purpose, either based on a nonlocal averaging (Pijaudier-Chabot and Bažant, 1987), gradient plasticity theories (Aifantis, 1984) or based on micromorphic media (Germain, 1973) of which many specific cases can be derived. The most famous of these cases is the micropolar continuum, better known as the Cosserat medium (Cosserat and Cosserat, 1909). Here, the local second gradient paradigm (Chambon and Caillerie, 1999; Germain, 1973; Matsushima et al., 2002) is chosen, which is a specific case of micromorphic medium in which the microkinematic gradient ν_{ij} is constrained to be equal to the macro displacement gradient $\partial u_i/\partial x_j$. The weak form balance equation can be written with Lagrange multipliers to avoid the use of C^1 shape functions for the displacement fields (Chambon et al., 2001):

$$\int_{\Omega^t}\left(\sigma_{ij}^t\frac{\partial u_i^\star}{\partial x_k^t}+\Sigma_{ijk}^t\frac{\partial \nu_{ij}^\star}{\partial x_k^t}\right)d\Omega-\int_{\Omega^t}\lambda_{ij}\left(\frac{\partial u_i^\star}{\partial x_j^t}-\nu_{ij}^\star\right)d\Omega-\bar{W}_e^\star=0 \tag{1}$$

with $\bar{W}_e^\star$ the external virtual work as an effect of the boundary traction $\bar{t}$ and the boundary double traction $\bar{T}$. Superscripts ^{t} and * denote quantities at time t and virtual quantities respectively; σ_{ij}^t are the components of the Cauchy stress tensor, Σ_{ijk}^t are the components of the double stress tensor. In addition, the constraint on the microkinematical tensor $\boldsymbol{\nu}$, with components ν_{ij}, requires the additional balance equation with respect to the Lagrange multiplier fields λ_{ij}:

$$\int_{\Omega^t}\lambda_{ij}^\star\left(\frac{\partial u_i^t}{\partial x_j^t}-\nu_{ij}^t\right)d\Omega^t=0 \tag{2}$$

The balance equation for the fluid part of the problem is formulated without the gradient enhancement. In absence of sink terms and neglecting gravitational influences, this gives:

$$\int_{\Omega^t}\left(\dot{M}^t p^\star-m_i^t\frac{\partial p^\star}{\partial x_i^t}\right)d\Omega-\bar{R}_e^\star=0 \tag{3}$$

where m_i^t are the components of the fluid mass flux. The external virtual work $\bar{R}_e^\star$ is the combined effort of the boundary fluid mass flux $\bar{m}^t=m_i n_i$ (n_i being the components of the boundary normal outward vector $\vec{n}$) and possible sink terms Q^t. M is the specific mass of the fluid phase with $\dot{M}$ its time derivative and p is the pore pressure. The iterative search to a configuration Ω^t for which (1) to (3) hold entails looking for a configuration $\Omega^{\tau 2}$ that corrects for the residual terms $W_{res}^{\tau 1}$, $T_{res}^{\tau 1}$ and $R_{res}^{\tau 1}$ corresponding to (1), (2) and (3) respectively from a preceding test solution of configuration $\Omega^{\tau 1}$, using a full Newton-Raphson procedure. Development of the iterative procedure in an updated lagrangian formulation (with respect to configuration $\tau 1$), leads to the following combined expression of iterative update $\mathrm{d}\Omega$ between $\Omega^{\tau 1}$ and $\Omega^{\tau 2}$ (see Matsushima et al., 2002 and Collin et al., 2006 for full details):

$$\int_{\Omega^{\tau 1}}[U_{(x,y)}^{\star,\tau 1}][E^{\tau 1}][\mathrm{d}U_{(x,y)}^{\tau 1}]d\Omega=-W_{res}^{\tau 1}-T_{res}^{\tau 1}-R_{res}^{\tau 1} \tag{4}$$

The column vector $[\mathrm{d}U^{\tau 1}]$ contains subsequently the terms $\frac{\partial \mathrm{d}u_i^{\tau 1}}{\partial x_j^{\tau 1}}$, $\frac{\partial \mathrm{d}p^{\tau 1}}{\partial x_j^{\tau 1}}$, $\mathrm{d}p^{\tau 1}$, $\frac{\partial \mathrm{d}\nu_{ij}^{\tau 1}}{\partial x_k^{\tau 1}}$, $\mathrm{d}\nu_{ij}^{\tau 1}$ and $\mathrm{d}\lambda_{ij}^{\tau 1}$, with $\mathrm{d}[.]^{\tau 1}$ the difference between subsequent iterative test solutions $[.]^{\tau 1}$ and $[.]^{\tau 2}$. The 23×23 matrix $[E^{\tau 1}]$ can written as